ME141C: **Spring 2007**
MEMS **C.D. Meinhart**

Home Work 4

Due: 5 June 2007

AC ELECTROKINETICS FOR BIO-MEMS

Note: Instructions for this homework are available on class website.

PROBLEM:
REACTION ENHANCEMENT USING ELECTROTHERMAL EFFECT

INTRODUCTION

In the homework 2, you modeled a Bio-MEMS sensor which utilized a diffusion limited surface reaction for detecting an antigen. You saw the effect of various parameters like diffusivity, mean velocity, channel heights etc. on the response of the sensor. You found that the binding response can be enhanced by shrinking the channel dimension, by increasing the velocities or by increasing the diffusivities.

In real life, it is very difficult to implement these suggestions. Diffusivity of an antigen can not be increased beyond a limit. The channel dimensions can not be shrunk below a critical size. The increase in velocities requires a lot of power.

The natural question is how else we can improve the binding response of the sensor. AC electrokinetics proves to be a ray of hope in such cases. One of the AC electrokinetic phenomena is electrothermal effect. The electrothermal effect can be utilized to create swirling patterns inside the channel in such a manner that the antigen's transport to the binding surface is enhanced. Following figure shows an example of the flow pattern generated due to electrothermal effect. Our aim is to simulate these flow patterns in COMSOL and determine what advantage they offer in terms of binding response of the sensor.

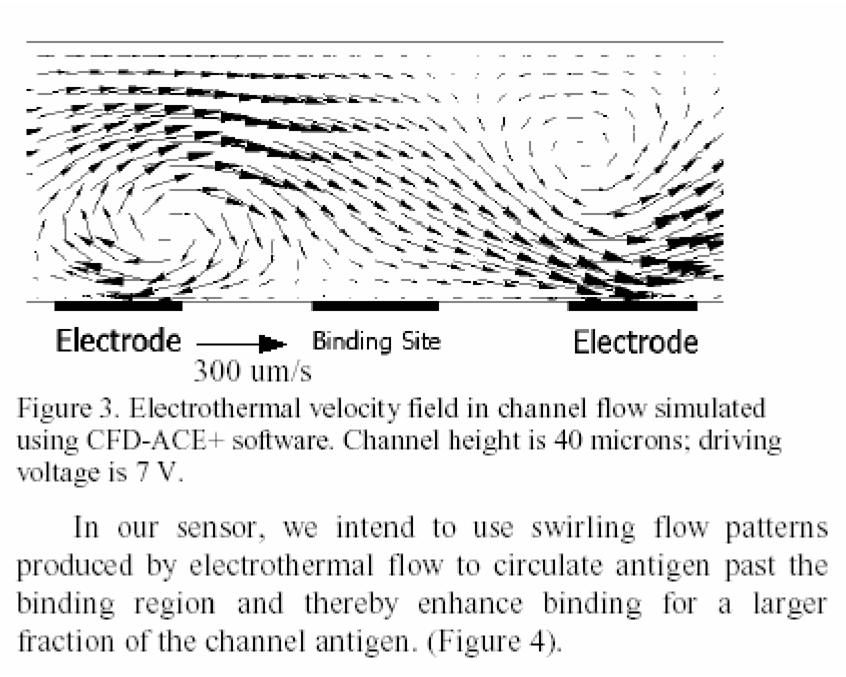


Figure 3. Electrothermal velocity field in channel flow simulated using CFD-ACE+ software. Channel height is 40 microns; driving voltage is 7 V.

In our sensor, we intend to use swirling flow patterns produced by electrothermal flow to circulate antigen past the binding region and thereby enhance binding for a larger fraction of the channel antigen. (Figure 4).

THEORY

Electrothermal effect is an AC electrokinetic phenomenon. It refers to a body force which acts on the fluid in presence of an <u>AC electric field</u> plus the <u>spatial gradients of conductivity and permittivity.</u> One should note that the conductivity and permittivity are temperature dependent properties and their spatial gradients are produced automatically by the non uniform Joule heating of the fluid in presence of the non uniform electric field.

The electric field is governed by the following equations

$$\nabla^2 V = 0 \tag{1}$$

$$\vec{E} = -\nabla V \tag{2}$$

The expression for the Joule heating is given by

$$q = \sigma E^2$$

The temperature of the fluid is governed by the following equation

$$\rho Cp \frac{DT}{Dt} = k\nabla^2 T + \sigma E^2 \tag{3}$$

Note that the Joule heating term appears as a source term on the right hand side. Once the temperature field is known, one can find the spatial gradients of the conductivity and permittivity as follows

$$\nabla\varepsilon = (\partial\varepsilon/\partial T)\nabla T \tag{4}$$

$$\nabla\sigma = (\partial\sigma/\partial T)\nabla T\ . \tag{5}$$

Here, T is the temperature of the fluid. For water, $(1/\varepsilon)(\partial\varepsilon/\partial T) = -0.4\%$ and $(1/\sigma)(\partial\sigma/\partial T) = +2\%$ per degree Kelvin.

The electrothermal body force depends on these spatial gradient and is expressed as

$$\vec{f}_E = -0.5\left[\left(\frac{\nabla\sigma}{\sigma} - \frac{\nabla\varepsilon}{\varepsilon}\right)\cdot\vec{E}_{rms}\frac{\varepsilon\vec{E}_{rms}}{1+(\omega\tau)^2} + 0.5\,|E_{rms}|^2\,\nabla\varepsilon\right] \tag{6}$$

This body force leads to the swirling motion in the fluid. The fluid motion can be solved from the well known Navier Stokes equation with the body force term added on the right hand side.

$$\rho\frac{\partial\vec{u}}{\partial t} + \rho\vec{u}\cdot\nabla\vec{u} = \eta\nabla^2\vec{u} - \nabla p + \vec{f}_E \tag{7}$$

Assuming no effective advection and steady state condition, this equation can be simplified to

$$\eta\nabla^2\vec{u} - \nabla p + \vec{f}_E = 0 \tag{8}$$

The mass-conservation equation for an incompressible fluid can be written as

$$\nabla\cdot\vec{u} = 0 \tag{9}$$

Now that you know the velocity field generated by the electrothermal forces, you can find its effect on the reaction binding. The transport of the antigen to the binding surface is governed by the following equation

$$\frac{\partial C}{\partial t} + \vec{u}\cdot\nabla C = D\nabla^2 C \tag{10}$$

One can note that the velocity appears in the advection terms on the left hand side and helps in transporting the antigen which is otherwise transported through diffusion only.

Once the antigen reaches the binding surface, it is bound to the antibody ligand. The time rate of change of antigen bound to the immobilized antibody is equal to the rate of association minus the rate of dissociation

$$\frac{\partial B}{\partial t} = k_{on}C_w(R_T - B) - k_{off}B \tag{11}$$

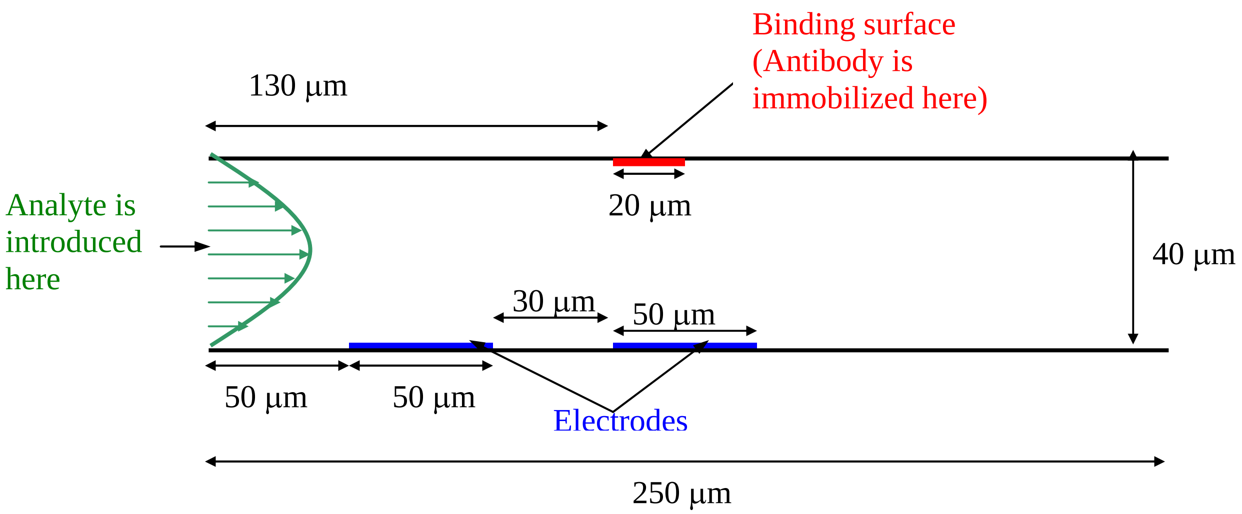
The rate of antigen binding to immobilized antibody, $\partial B/\partial t$ must be balanced by the diffusive flux of antigen at the binding surface, $y = 0$ such that

$$\frac{\partial B}{\partial t} = D\left.\frac{\partial C}{\partial y}\right|_{y=0} \tag{12}$$

SIMULATION

1. Model the following geometries in Comsol 3.2 by using your knowledge from Homework #2. Your final goal is to model the AC electrokinetically enhanced reactions i.e. the physics described above (eqns 1 to 12). Add the required physics modes, appropriate constants, expressions and coupling variables. Define subdomain settings and boundary conditions appropriately.

   Assume the following
   a) A 20 Volt rms is applied to the electrodes. (i.e., +10 Volt at the left electrode and –10 Volt at the right). This is how a AC electric field can be modeled easily.
   b) The electrodes are perfect heat sinks i.e. they are isothermal with the ambient (i.e. T=0).
   c) The flow is parabolic at the entrance with a centerline velocity of 1.5e-4 m/s.
   d) All the constants related to the binding reaction process are the same as homework #2.



2. The electrodes at the bottom wall will be used for generating an AC electric field inside the channel. Show the electric potential and electric field lines.
3. Due to Joule heating, the temperature of the fluid will increase non-uniformly. Show the temperature field inside the channel in steady state. Is the temperature field spatially non uniform? Why is this non-uniformity important?
4. The temperature gradients give rise to electrothermal forces. Show how the flow patterns look like under these forces. How is the flow pattern different from usual channel flow which you did in HW#2? How can this flow pattern help in reaction binding?
5. Similar to HW#2, solve for the time dependent binding reaction process with these flow patterns. Show the concentration field inside the channel at t=2 minute. Plot the B_ave vs. t curve and find the reaction rate.
6. Now repeat the steps 2 to 5 with 0 volt applied to each electrode. This will give you a case without electrothermal effect. Compare the reaction rates of both the cases. How

much improvement do you find in reaction rate within the first 2 minutes due to the electrothermal effect? How much improvement do you find in the average bound concentration in 2 minutes?

7. <u>Optimization of the sensor location</u>
   Do you think that the binding response can be further improved by selecting a more appropriate location for the binding surface? By looking at the flow pattern inside the channel, decide better locations for the binding surface. You can try placing the surface between the electrodes at the bottom wall. You may also try some other location on the top wall. Optimize the location of the sensor and show B_ave vs. t curves for all the locations which you tried.